

**Anisotropic Heisenberg ferromagnetic model in two dimensions**

E. E. Reinehr and W. Figueiredo

*Departamento de Física, Universidade Federal de Santa Catarina, 88040-900, Florianópolis, Santa Catarina, Brazil*  
(Received 17 February 1995)

We have studied the behavior of the magnetization as a function of temperature of a two-dimensional anisotropic Heisenberg ferromagnetic model within the Green's-function formalism. We have shown that our magnetization curves do not present any plateau in the limit of very small anisotropies, as predicted by the real-space renormalization-group calculations. We compare our results with the recent experimental measurements performed on quasi-two-dimensional films. We also consider the asymptotic spin-wave limit to explain the low-temperature experimental data.

**I. INTRODUCTION**

The low-dimensional magnetic systems have received a great deal of attention in recent years. Several theoretical techniques have been employed to understand these systems: high-temperature series expansions,<sup>1</sup> Monte Carlo simulations,<sup>2</sup> renormalization group,<sup>3</sup> and Green's-function formalism<sup>4</sup> are some of the methods used in these studies. In this work we apply the formalism of Green's function to calculate the magnetization as a function of temperature of the anisotropic Heisenberg model. Our motivation to study this problem is the recent real-space renormalization-group calculation,<sup>5</sup> which shows that, in the limit of small anisotropies, the magnetization curves exhibit a plateau as a function of temperature. These calculations were used to fit the experimental data of Mauri *et al.*<sup>6</sup> on quasi-bidimensional ferromagnetic systems. We show that, with the aid of Green's-function formalism, the plateau does not appear and we are able to fit the experimental data of Mauri *et al.*<sup>6</sup> We also discuss the spin-wave limit and its relation with the experimental data mentioned above.

**II. CALCULATIONS**

We consider the following Hamiltonian of a two-dimensional anisotropic Heisenberg ferromagnetic model:

$$H = - \sum_{\langle ij \rangle} [W(S_i^+ S_j^- + S_i^- S_j^+) + JS_i^z S_j^z], \quad (1)$$

where the summation is over the nearest-neighbor pairs of  $\frac{1}{2}$  spins,  $J$  is the exchange coupling between neighboring spins, and  $W/J$  measures the degree of exchange anisotropy. When  $W/J$  ranges from 0 to 1, we go from the Ising to the Heisenberg ferromagnetic model.

The equation of motion for the Fourier transform of the Green's function<sup>7</sup> can be written as

$$EG_{\mathbf{g}\mathbf{m}}(E) = \frac{1}{2\pi} \langle [S_{\mathbf{g}}^+, S_{\mathbf{m}}^-] \rangle + \langle \langle [S_{\mathbf{g}}^+(t), H]; S_{\mathbf{m}}^-(0) \rangle \rangle_E, \quad (2)$$

where  $\mathbf{g}$  and  $\mathbf{m}$  are two lattice sites, and  $G_{\mathbf{g}\mathbf{m}}(E)$  is the Fourier transform of the Green's function  $\langle \langle S_{\mathbf{g}}^+(t), S_{\mathbf{m}}^-(t') \rangle \rangle$ .

In order to solve the system of equations generated by Eq. (2), we need to break the chain of Green's functions. In this paper we consider the simplest decoupling scheme, the random-phase approximation (RPA), where the longitudinal and transversal components of the spin operators at different sites of the lattice are uncorrelated,<sup>8</sup> that is,

$$\langle \langle S_{\mathbf{g}}^z S_{\mathbf{i}}^+; S_{\mathbf{m}}^- \rangle \rangle = \langle S_{\mathbf{g}}^z \rangle \langle \langle S_{\mathbf{i}}^+; S_{\mathbf{m}}^- \rangle \rangle. \quad (3)$$

Taking into account the translational symmetry of the lattice we can write that

$$G_{\mathbf{g}\mathbf{m}}(E) = \frac{1}{N} \sum_{\mathbf{k}} G_{\mathbf{k}}(E) e^{ik(\mathbf{g}-\mathbf{m})}, \quad (4)$$

where the summation is over the set of  $\mathbf{k}$  vectors inside the first Brillouin zone. In this way we find that

$$G_{\mathbf{k}}(E) = \frac{\langle S^z \rangle}{\pi} \frac{1}{(E - E_{\mathbf{k}})}, \quad (5)$$

where

$$E_{\mathbf{k}} = 2z \langle S^z \rangle (J - W\gamma_{\mathbf{k}}) \quad (6)$$

is the magnon energy spectrum, and  $\gamma_{\mathbf{k}}$  is the structure factor of the lattice with coordination number  $z$ .

With the help of the spectral density function,<sup>8</sup> defined as

$$J(E) = \frac{i}{e^{E/k_B T} - 1} \lim_{\epsilon \rightarrow 0} [G(E + i\epsilon) - G(E - i\epsilon)], \quad (7)$$

we can find the equilibrium correlation function  $\langle S^- S^+ \rangle$ , through

$$\langle S^- S^+ \rangle = \int_{-\infty}^{+\infty} J(E) e^{E/k_B T} dE. \quad (8)$$

As for spin  $S = \frac{1}{2}$  we can write that

$$\langle S^z \rangle = \frac{1}{2} - \langle S^- S^+ \rangle, \quad (9)$$

we finally arrive at the following expression for the magnetization:

$$\frac{1}{2\langle S^z \rangle} = \frac{1}{N} \sum_{\mathbf{k}} \coth \left[ \frac{\beta E_{\mathbf{k}}}{2} \right]. \quad (10)$$

By replacing the summation by an integral over the two-dimensional Brillouin zone, we can write that

$$\frac{1}{2\langle S^z \rangle} = \frac{v}{(2\pi)^2} \int_{\text{ZB}} \coth \left[ \frac{\beta E_{\mathbf{k}}}{2} \right] d^2\mathbf{k}, \quad (11)$$

where  $v$  is the volume of the unitary cell. This equation gives us the magnetization as a function of temperature and can be solved self-consistently.

### III. RESULTS

In the region of very low temperatures, that is, for

$$2zJ\langle S^z \rangle / k_B T \gg 1$$

and considering a square lattice of lattice spacing  $a$ , where

$$\gamma_{\mathbf{k}} = \frac{1}{2} [\cos(k_x a) + \cos(k_y a)], \quad (12)$$

we can expand the integral, in Eq. (11), in a power series. After some algebraic manipulations we obtain the following asymptotic expansion:

$$\langle S^z \rangle = \frac{1}{2} - \frac{1}{\pi} \frac{\tau}{1-\Delta} Z_1 \left[ \frac{\Delta}{\tau} \right] - \frac{1}{2\pi} \left[ \frac{\tau}{1-\Delta} \right]^2 Z_2 \left[ \frac{\Delta}{\tau} \right] - \dots, \quad (13)$$

where we have defined that

$$Z_n \left[ \frac{\Delta}{\tau} \right] = \sum_{l=1}^{\infty} \frac{\exp(-l\Delta/\tau)}{l^n}, \quad (14)$$

with  $\Delta = 1 - W/J$ , and  $\tau = k_B T / zJ$  is the reduced temperature.

As the energy spectrum has a gap at  $\mathbf{k}=0$ , which depends on the magnitude of the anisotropy  $\Delta$ , the magnetization decreases exponentially at very low temperatures for any value of the gap, except at the singular point  $\Delta=0$ . For this particular value, the two-dimensional integral, given in Eq. (11), diverges, and the isotropic Heisenberg ferromagnetic model cannot sustain a long-range order at finite temperatures, according to the Mermin and Wagner theorem.<sup>9</sup>

On the other hand, near the critical temperature, where  $\langle S^z \rangle$  goes to zero, we can again expand the argument into the integral, in Eq. (11), because now it is very small. In this case, it is easy to show that

$$\langle S^z \rangle = \left[ \frac{3\tau}{A} \left[ 1 - \frac{\tau}{\tau_c} \right] \right]^{1/2}, \quad (15)$$

where

$$\frac{1}{\tau_c} = \frac{2v}{(2\pi)^2} \int_{\text{ZB}} \frac{d^2\mathbf{k}}{[1 - (W/J)\gamma_{\mathbf{k}}]} \quad (16)$$

and

$$A = \frac{2v}{(2\pi)^2} \int_{\text{ZB}} \left[ 1 - \frac{W}{J} \gamma_{\mathbf{k}} \right] d^2\mathbf{k}. \quad (17)$$

As we can see, the Green's-function formalism, in the RPA scheme, gives the classical exponent  $\beta = \frac{1}{2}$  for the magnetization.

In Fig. 1, we show the behavior of the magnetization as a function of temperature for different values of the anisotropy. These curves are obtained by solving self-consistently Eq. (11) for each value of temperature and of the anisotropy parameter. In order to perform these calculations we have replaced the integration over  $\mathbf{k}$  inside the first Brillouin zone by a discrete sum of highly symmetric set of special points. We have taken three million points inside the first Brillouin zone after extending the method of generating special points provided by Chadi and Cohen.<sup>10</sup> Even for the quasi-isotropic Heisenberg ferromagnetic model, curve  $F$ , we do not observe any plateau, as foreseen by the real-space renormalization-group calculations.<sup>5</sup> In Fig. 2 we exhibit the curve of critical temperature as a function of anisotropy. As to be expected, when  $W/J \rightarrow 1$ , the critical temperature goes to zero.

Finally, in Fig. 3, we apply our results to the experimental points of Mauri *et al.*<sup>6</sup> for the uncoupled Permalloy film of 1.6 monolayer thick. Our curve was constructed by taking  $\Delta=0.2$  and  $J_s/J_b=0.66$ , where  $J_s$  and  $J_b$  are the surface and bulk exchange couplings of the Permalloy film, respectively. Our results fit reasonably well the experimental data in the range of temperatures considered. Mauri *et al.*<sup>6</sup> have pointed out that the spin-wave calculations do not work very well for this system. As we know, the spin-wave theory, gives asymptotic expansions, like that in Eq. (13), which are valid only in the range of very small temperatures, that is, for

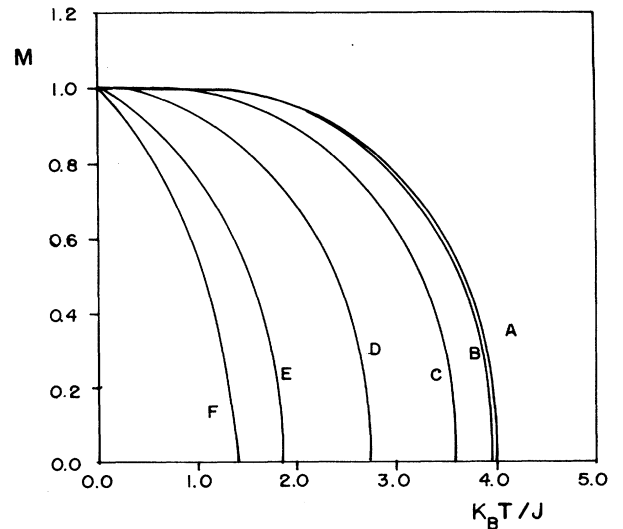


FIG. 1. Spontaneous magnetization curves for the anisotropic Heisenberg ferromagnetic model. Here  $\Delta = 1 - W/J$  measures the degree of exchange anisotropy. Curve  $A$  ( $\Delta = 1.0$ ),  $B$  ( $0.8$ ),  $C$  ( $0.4$ ),  $D$  ( $0.1$ ),  $E$  ( $0.01$ ), and  $F$  ( $0.001$ ).

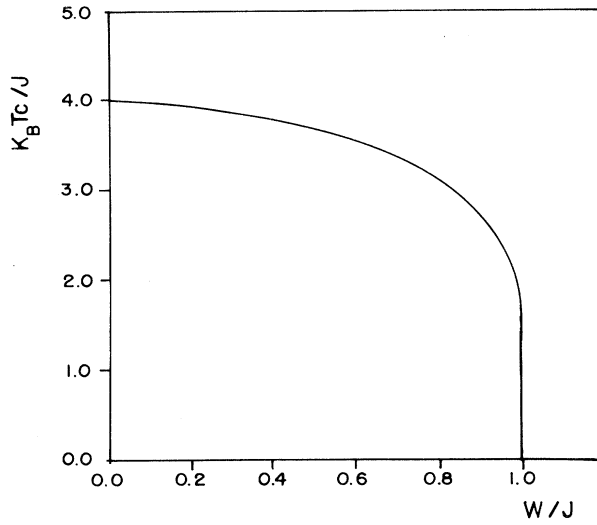


FIG. 2. Reduced critical temperature of the anisotropic Heisenberg ferromagnetic model as a function of the ratio  $W/J$  that measures the degree of exchange anisotropy.

$T \ll T_c$ , where  $T_c$  is the critical temperature. However, the critical temperature of the Permalloy film is about 340 K, and the lower measurement was performed at 80 K, which corresponds to 24% of the surface critical temperature of the Permalloy film. Due to this fact, we agree with Mauri *et al.*,<sup>6</sup> that the spin-wave expansions are not suitable to fit their experimental data. However, as the Green's-function formalism covers all range of temperatures, it was possible to fit their experimental data. As a matter of comparison we also have plotted in the same figure the real-space renormalization-group calculation.<sup>5</sup>

#### IV. CONCLUSIONS

In this work we have applied the Green's-function method to find the magnetization as a function of temperature for the anisotropic Heisenberg ferromagnetic mod-

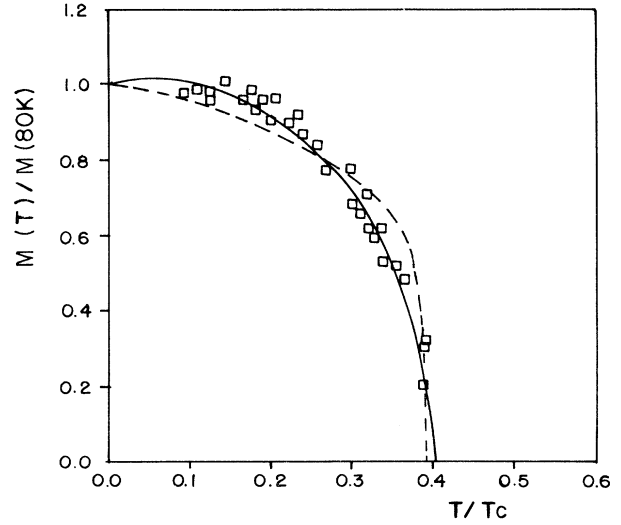


FIG. 3. Reduced magnetization as a function of reduced temperature. The continuous curve is our Green's-function calculation, the dashed line is the real-space renormalization-group result (Ref. 5), and the small squares are the experimental data (Ref. 6) of 1.6 monolayers of Permalloy. We have taken  $J_s/J_b = 0.66$ ,  $\Delta = 0.20$ , and  $T_c$  is the bulk critical temperature of Permalloy.

el. We have shown that the magnetization decreases smoothly towards the critical temperature for any value of the anisotropy parameter. This behavior is different from that observed in the real-space renormalization calculations, where a plateau appears in the magnetization curves for small values of the exchange anisotropy. Our results also fit reasonably well the recent magnetization data obtained for a two-dimensional Permalloy film.

#### ACKNOWLEDGMENTS

We would like to acknowledge the Brazilian agencies CNPq and FINEP for the financial support.

<sup>1</sup>K. Binder and P. C. Hohenberg, Phys. Rev. B **9**, 2194 (1974).

<sup>2</sup>K. Binder and D. P. Landau, Phys. Rev. Lett. **52**, 318 (1984).

<sup>3</sup>A. M. Mariz, U. M. S. Costa, and C. Tsallis, Europhys. Lett. **3**, 27 (1987).

<sup>4</sup>J. N. B. de Moraes and W. Figueiredo, J. Phys. Condens. Matter **5**, 3809 (1993).

<sup>5</sup>A. Chame, J. Phys. Condens. Matter **3**, 9115 (1991).

<sup>6</sup>D. Mauri, D. School, H. C. Siegmann, and E. Kay, Phys. Rev. Lett. **62**, 1900 (1989).

<sup>7</sup>D. N. Zubarev, Sov. Phys. Usp. **3**, 320 (1960).

<sup>8</sup>S. V. Tyablikov, *Methods in the Quantum Theory of Magnetism* (Plenum, New York, 1967).

<sup>9</sup>N. D. Mermin and H. Wagner, Phys. Rev. Lett. **7**, 5212 (1973).

<sup>10</sup>D. J. Chadi and M. L. Cohen, Phys. Rev. B **8**, 5747 (1973).